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Résumé - Un schéma général est dérivé pour calculer des densités de niveaux à m particules et n trous des fermions pour tout Hamiltonien à particules indépendantes en tenant compte du principe de Pauli. Cette technique est appliquée pour obtenir les densités de niveaux de l'oscillateur harmonique isotropique à trois dimensions semiclassiquement dans l'approximation de Thomas-Fermi.

Abstract - A general scheme is derived to calculate m-particle n-hole fermion level densities for any single particle Hamiltonian taking into account Pauli exclusion. This technique is applied to obtain level densities of the three dimensional isotropic Harmonic Oscillator semiclassically in the Thomas-Fermi approach.

1 - INTRODUCTION -

It has been shown recently [1] that the usual Thomas-Fermi (TF) approach [2], which is a semiclassical treatment, yields average 1-particle 1-hole and 2-particle 2-hole level densities, of an isotropic Harmonic Oscillator, which are in a very good agreement to the exact quantum mechanical level densities. We develop a general scheme which permits to calculate exactly arbitrary m-particle n-hole excitations for any type of single particle Hamiltonians. We explicitly take into account the Pauli exclusion principle for fermions. Encouraged by the above mentioned TF results, we use our scheme to calculate all m-particle n-hole level densities up to m,n = 3.

Level densities with equal number of particles and holes are of interest for instance in the study of precompound reactions and of the spreading widths of giant resonances [3,4]. On the other hand, the level densities associated with unequal number of particles and holes find their application in the calculation of shell model optical potentials [2].

In the next section we derive an iteration formula to calculate the m-particle n-hole level densities. In section 3 we apply this scheme to the case of an isotropic three dimensional Harmonic oscillator. We obtain analytical results in the TF approach.

2 - DERIVATION OF AN ITERATION FORMULA FOR MANY-PARTICLE MANY-HOLE LEVEL DENSITIES -

The definition of the exact m-particle n-hole level density for fermions as a function of the energy E is :

$$g_{mp\,nh}(E) = \sum_{\substack{p_1<\cdots<p_m \\ h_1<\cdots<h_n}} \delta\left(E - \sum_{p=p_1}^{p_m} \varepsilon_p + \sum_{h=h_1}^{h_n} \varepsilon_h\right) \qquad (2.1)$$

where the m+n fold sum outside of the Dirac delta function δ extends over all particle states (labelled by the indexes p_1 through p_m) with the restriction $p_1<\ldots<p_m$,

and similarly for the hole states h_i. The restrictions $p_1<\ldots< p_m$, and $h_1<\ldots<h_n$ are to avoid multiple counting of the same terms and to honor the Pauli exclusion principle. The ε_i are the eigenvalues of the single particle Hamiltonian H.

Equation (2.1) can be rewritten as :

$$g_{mp\ nh}(E) = \sum_{\substack{\mu_1<\ldots<\mu_m \\ \nu_1<\ldots<\nu_n}} \langle\mu_1,\ldots\mu_m,\nu_1,\ldots\nu_n| \prod_{\mu=\mu_1}^{\mu_m} \theta(H_\mu-\varepsilon_F) \prod_{\nu=\nu_1}^{\nu_n} \theta(\varepsilon_F-H_\nu)\delta(E-\sum_{\mu=\mu_1}^{\mu_m}\varepsilon_\mu + \sum_{\nu=\nu_1}^{\nu_n}\varepsilon_\nu)$$

$$|\mu_1,\ldots\mu_m,\nu_1,\ldots\nu_n\rangle \qquad (2.2)$$

By introducing the proper step functions θ, the particle states are guaranteed to lie above the fermi energy ε_F, and the hole states below. We replaced the summation indices p_i and h_i by μ_i and ν_i to indicate that each of them runs now over all particle and hole states. We introduced also the product eigenstates with the property

$$H_i\ |\mu_1\ldots\mu_m,\ \nu_1\ldots\nu_n\rangle = \varepsilon_i\ |\mu_1\ldots\mu_m,\ \nu_1\ldots\nu_n\rangle \qquad (2.3)$$

where i is of the set $\{\mu_1,\ldots\mu_m,\ \nu_1,\ldots\nu_n\}$.

A convenient representation of the level density is obtained by applying a Fourier transform ($E \to t$, with the definition : $\beta = \frac{it}{\hbar}$) to eq.(2.2) :

$$G_{mp\ nh}(\beta) \equiv \int_{-\infty}^{\infty} dE\ e^{-\beta E}\ g_{mp,nh}(E) = A_m(\beta).B_n(\beta) \qquad (2.4)$$

i.e. the result factorizes into a particle component

$$A_m(\beta) \equiv \sum_{\mu_1<..<\mu_m} \langle\mu_1,..\mu_m| \prod_{\mu} \theta(H_\mu-\varepsilon_F)\ e^{-\beta\sum H_\mu}|\mu_1,\ldots\mu_m\rangle \qquad (2.5)$$

and a hole component

$$B_n(\beta) \equiv \sum_{\nu_1<\ldots<\nu_n} \langle\nu_1,\ldots\nu_n| \prod_{\nu} \theta(\varepsilon_F-H_\nu)\ e^{+\beta\sum H_\nu}|\nu_1,\ldots\nu_n\rangle \qquad (2.6)$$

Note that if the sums in eqs.(2.5) and (2.6) were unrestricted, one could write A_m and B_n simply as traces. However, it is possible to express A_m and B_n in terms of traces, by observing the following. A restricted sum over two indices of a function f can be written as an unrestricted sum minus a sum over the diagonal terms and divided by two to take into account double counting. To simplify our notation, we define

$$f(\mu) \equiv \langle\mu|\theta(H_\mu-\varepsilon_F)\ e^{-\beta H_\mu}|\mu\rangle \qquad (2.7)$$

and note that eq.(2.5) for two particles can then be written as

$$\sum_{\mu_1<\mu_2} f(\mu_1)f(\mu_2) = \frac{1}{2}\left[\sum_{\mu_1,\mu_2} f(\mu_1)f(\mu_2) - \sum_{\mu_1} f^2(\mu_1)\right] \qquad (2.8)$$

Similarly, in the case of three indices, we have

$$\sum_{\mu_1<\mu_2<\mu_3} f(\mu_1)f(\mu_2)f(\mu_3) = \frac{1}{3!}\left[\sum_{\mu_1,\mu_2,\mu_3} f(\mu_1)f(\mu_2)f(\mu_3) - 3\sum_{\mu_1,\mu_2} f^2(\mu_1)f(\mu_2) + 2\sum_{\mu_1} f^3(\mu_1)\right] \qquad (2.9)$$

The sum with a negative sign arises from the fact that we have to subtract from the unrestricted sum the terms with $\mu_1=\mu_2$, $\mu_1=\mu_3$ and $\mu_2=\mu_3$. The last sum over terms with $\mu_1=\mu_2=\mu_3$ has to be added twice, since the three sums we subtract each

contain these terms, but the unrestricted sum only contains them once. The factor $\frac{1}{3!}$ comes about because one has to compensate for overcounting, i.e. terms with $\mu_1>\mu_2$ etc., which occur 3! times for three indices.

Note, that in eqs.(2.8) and (2.9) the sums on the right hand side are now unrestricted and therefore can be written as traces. For an arbitrary number of indices we obtain from combinatorics the following iteration formulae for a new set of functions $A_m^{(\ell)}$ and $B_n^{(\ell)}$ (defined as

$$A_m^{(\ell)} = m! \sum_{\mu_1<\ldots\mu_m} \langle \mu_1,..\mu_m | \pi_\mu \theta(H_\mu - E_F) e^{-\beta\Sigma H_\mu} e^{-\beta\ell H_{\mu_1}} | \mu_1,..\mu_m \rangle \tag{2.10}$$

and similarly for $B_n^{(\ell)}$):

$$A_m^{(\ell)}(\beta) = A_1^{(\ell)}(\beta).(A_1^{(o)}(\beta))^{m-1} - \sum_{k=2}^{m} \binom{m}{k} A_{m-k+1}^{(k+\ell-1)}(\beta) \quad \text{for } m \geq 2 \tag{2.11}$$

$$B_n^{(\ell)}(\beta) = B_1^{(\ell)}(\beta).(B_1^{(o)}(\beta))^{n-1} - \sum_{k=2}^{n} \binom{n}{k} B_{n-k+1}^{(k+\ell-1)}(\beta) \quad \text{for } n \geq 2 \tag{2.12}$$

with the initial definitions

$$A_1^{(\ell)}(\beta) \equiv \mathrm{tr}\ \{\theta(H-\varepsilon_F)\ e^{-(\ell+1)\beta H}\} \tag{2.13}$$

$$B_1^{(\ell)}(\beta) \equiv \mathrm{tr}\ \{\theta(\varepsilon_F-H)\ e^{+(\ell+1)\beta H}\} \tag{2.14}$$

The Fourier transformed level density is then

$$G_{mpnh}(\beta) = A_m(\beta).B_n(\beta) = \frac{1}{m!} A_m^{(o)}(\beta).\ \frac{1}{n!}\ B_n^{(o)}(\beta) \tag{2.15}$$

The functions $A_m^{(\ell)}$ and $B_n^{(\ell)}$ are completely determined by the iteration procedure, eqs.(2.10) through (2.14), as is the level density, eq.(2.15). Note that level densities of the form g_{opnh} and g_{mpoh} are obtained by setting $A_o(\beta) = 1$ or $B_o(\beta) = 1$, respectively, as follows immediately from eq.(2.1).

The above equations are valid for level densities of any (single particle) Hamiltonian. We emphasize that in the case $\ell = o$, the sums which are subtracted in eqs.(2.11) and (2.12) are the correction terms due to the Pauli exclusion principle (because they subtract terms with equal indices, compare with eqs.(2.8) and (2.9)). We now proceed to apply these equations to a particular case.

3 - SEMICLASSICAL LEVEL DENSITIES OF THE HARMONIC OSCILLATOR -

We consider the three dimensional isotropic Harmonic Oscillator Hamiltonian.

$$H_i = \frac{p_i^2}{2m} + \frac{1}{2} m \omega_o^2 r_i^2 \tag{3.1}$$

The semiclassical (Thomas-Fermi) approximation [2] is obtained by replacing the operator H_i by its classical counterpart and the traces in eqs.(2.11) - (2.15) by integrations over phase space, i.e..

$$\mathrm{tr}_i \to d \cdot \frac{1}{(2\pi\hbar)^3} \int d^3r_i\ d^3p_i \tag{3.2}$$

where d denotes the spin degeneracy of fermions, d = 2. In this work, we do not take into account isospin degeneracy.

In the semiclassical approximation eqs.(2.13) and (2.14) become

$$A_1^{(\ell)}(\beta) = \frac{d}{(\hbar\omega_o)^3} e^{-(\ell+1)\beta\varepsilon_F}\left(\frac{\varepsilon_F^2}{2(\ell+1)\beta} + \frac{\varepsilon_F}{(\ell+1)^2\beta^2} + \frac{1}{(\ell+1)^3\beta^3}\right) \tag{3.3}$$

$$B_1^{(\ell)}(\beta) = \frac{d}{(\hbar\omega_o)^3}\left[e^{+(\ell+1)\beta\varepsilon_F}\left(\frac{\varepsilon_F^2}{2(\ell+1)\beta} - \frac{\varepsilon_F}{(\ell+1)^2\beta^2} + \frac{1}{(\ell+1)^3\beta^3}\right) - \frac{1}{(\ell+1)^3\beta^3}\right] \tag{3.4}$$

Then the level densities $g_{mpnh}(E)$ are obtained with the help of iteration formulae eqs.(2.11) and (2.12) and ^{mpnh} by an inverse Fourier transform of eq.(2.15), which can be done analytically, since it involves only terms of the type $e^{-\mu\beta\varepsilon_F}\,\beta^{-\nu}$ which transform to $\theta(E-\mu\varepsilon_F)\,(E-\mu\varepsilon_F)^{\nu-1}/(\nu-1)!$ (ν,μ intergers, $\nu>0$, $\mu=0, \pm1,\ldots$).

For the case of one-particle one-hole and two-particle two-hole excitations the level densities have been derived in ref.[1]* already. For higher order level densities the analytical expressions become prohibitively lengthy to be calculated by hand. Therefore we made use of the computer code REDUCE [5], which allows for analytical treatment of lengthy expressions.

We now discuss some of the results. We are not going to compare the semiclassical level densities to the exact quantum mechanical ones, since it has been shown in refs.[1] and [6] that already for g_{1p1h} and g_{2p2h} the overall agreement of the semiclassical results with the exact ones is excellent.

3.1. The Role of the Pauli Exclusion Principle -

First we show the role of the Pauli exclusion principle. In Fig. 1, the lower curve shows the complete level density g_{3p3h} as a function of the energy, whereas the upper curve represents the direct terms, i.e. is not corrected for the Pauli principle (see the remark at the end of Section 2). The deviation is of the order of 35% at $E/\hbar\omega_o = 5$, and of 17% at $E/\hbar\omega_o = 50$ in this case. It gets smaller for higher energies. It is also smaller for lower order excitations (e.g. for g_{2p2h} it is 7% at $E/\hbar\omega_o = 5$ and 5% at $E/\hbar\omega_o = 50$).

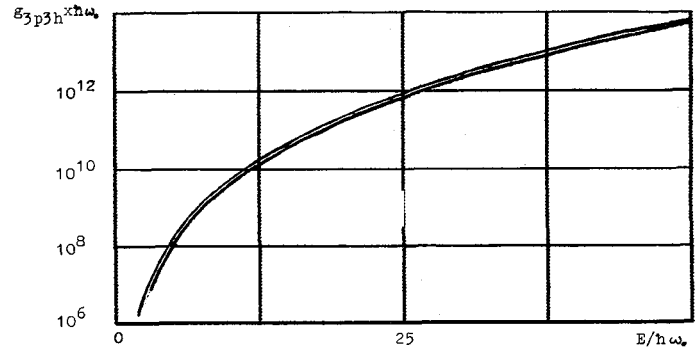


Fig.1- The effect of the Pauli principle on the semiclassical 3-particle 3-hole level density g_{3p3h} as a function of energy E, in units of $\hbar\omega_o$, which is the Harmonic oscillator constant. The upper curve is calculated without taking Pauli exclusion into account, the lower one is the full level density obeying the Pauli principle. The curves in all figures are for 40 fermions (no isospin considered).

*Footnote : In Ref.[1] g_{1p1h} is too small by a factor of 2 and g_{2p2h} by a factor of 4.

3.2. Level Densities with Equal Number of Particles and Holes -

We show the level densities g_{1p1h} (lowest curve), g_{2p2h} (middle curve) and g_{3p3h} in Fig. 2. As should be expected, the level density curves differ by orders of magnitude, since the available phase space increases drastically with the order of particle-hole excitations.

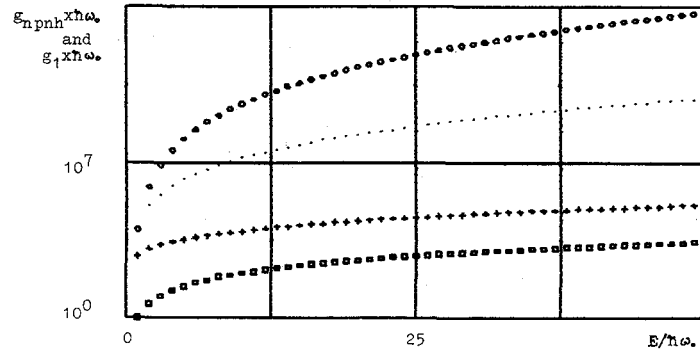


Fig.2 - The excitation level densities g_{1p1h} (crosses), g_{2p2h} (dots) and g_{3p3h} (uppermost curve). The lowest curve indicates the one-particle level density g_1

Depositing a given amount of energy E in a system of many particles in a potential excites all n-particle n-hole states which are above their respective thresholds. Therefore we show the sum

$$g(E) \equiv g_{1p1h}(E) + g_{2p2h}(E) + g_{3p3h}(E) \tag{3.5}$$

in Fig.3 and compare it to the well-known statistical formula [7]

$$g_{Stat}(E) = \left(\frac{2\varepsilon_F}{N}\right)^{1/4} \frac{1}{12} E^{-5/4} \exp\left\{\left(\frac{4\pi^2 N}{\varepsilon_F} E\right)^{1/2}\right\} \tag{3.6}$$

where we calculate the Fermi energy ε_F semiclassically from the particle number N in the Harmonic Oscillator

$$\varepsilon_F = (3N)^{1/3} \hbar\omega_0 \tag{3.7}$$

The statistical prediction lies above the semiclassical sum for higher excitations, supposedly because we did not take into account excitations higher than 3-particle 3-hole. Although the diagram shows only excitations below 4 $\hbar\omega_0$, where there are no 4-particle 4-hole states allowed by quantum mechanics, we should note that the semiclassical results exhibit an average behavior. Therefore the g_{4p4h} level density does have a tail below its exact threshold and should be included in the sum (3.5), which we did not.

The number of states for an n-particle n-hole excitation is given by :

$$N_{npnh}(E) = \int_0^E dE' g_{npnh}(E') \tag{3.8}$$

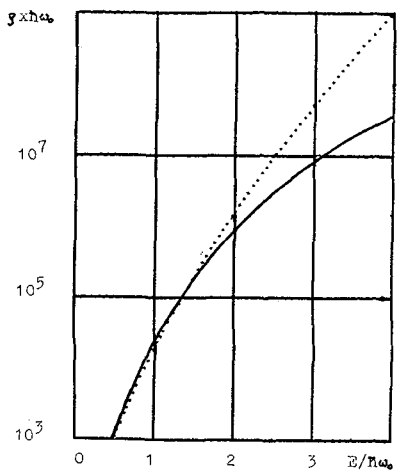


Fig.3 - The statistical excitation level density (see eq.(3.6)), dotted line, and the sum $g_{1p1h} + g_{2p2h} + g_{3p3h}$, full curve.

Since N_{1p1h} and N_{2p2h} are already shown in Ref.[**1**] we include the graph for N_{3p3h} for reference (Fig.4).

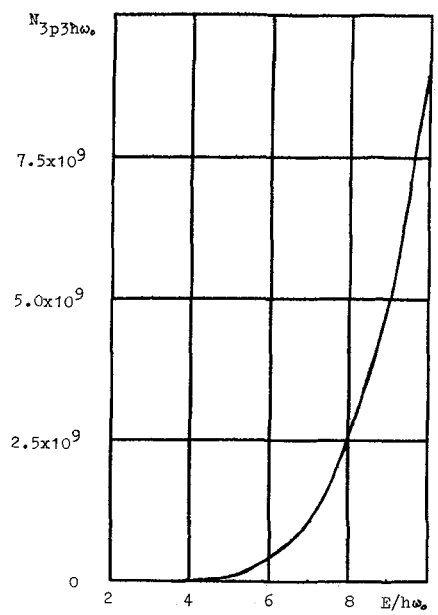


Fig.4 - The number of states for 3-particle 3-hole excitations, obtained by integrating $g_{3p3h}(E)$, eq.(3.8).

3.3. Particle Level Densities -

We proceed to consider the single particle level density, defined in anology to eq.(2.1) as

$$g_1(E) = \sum_i \delta (E - \varepsilon_i) \qquad (3.9)$$

(The integral (3.8) performed on g_1 gives then eq.(3.7), since $N = N_1(\varepsilon_F)$). Eq. (3.9) can be written instead as

$$g_1(E) = g_{1p0h}(E) + g_{0p1h}(-E) \qquad (3.10)$$

the minus sign being necessary since hole energies are negative. The term $g_{0p1h}(-E)$ contributes in the energy range o... ε_F, whereas $g_{1p0h}(E)$ contributes from ε_F to infinity. They match of course exactly at the fermi energy ε_F. The curve of g_1 is included in Fig.2 (it is the lowest one). In anology to eq. (3.10) we can define g_2 and g_3 which are shown in Fig.5. They decrease sharply at $2\varepsilon_F$ and $3\varepsilon_F$, respectively, the matching point of the two components of g_2 and of g_3. Although the level density g_1 for single particles is considerable at ε_F (see fig.2), the phase space for two particles or two holes, and three particles or three holes at ε_F per particle or hole is depleted, due to momentum conservation. The energy of g_2 and g_3 extends from 0 to infinity.

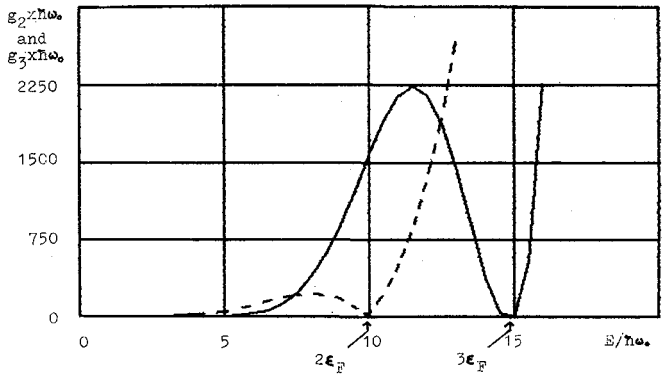


Fig.5 - The 2-particle and 3-particle level densities g_2 (dashed line) and g_3 (full line). The points on the energy axis with two times and three times the Fermi energy ε_F are indicated (see text for discussion). Level density g_1 is shown in Fig.2.

3.4. Level Densities with Unequal Number of Particles and Holes -

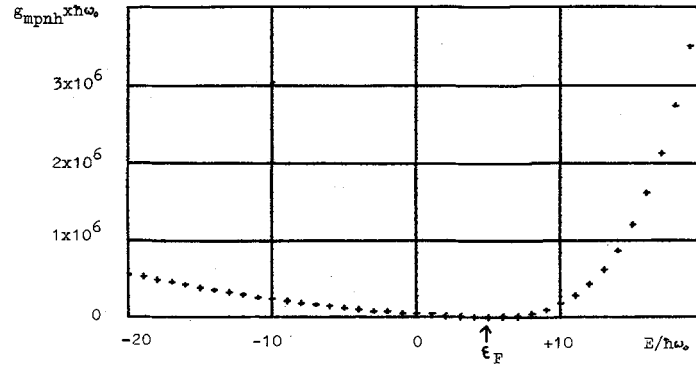
Finally, in Fig.6, we show m-particle n-hole level densities (for $m \neq n$ and $m, n \neq 0$), which are of interest in optical model calculations [2]. Again, we include $g_{mpnh}(E)$ and $g_{npmh}(-E)$ in one curve. The results are defined in the range $-\infty < E < +\infty$, and the level densities have again their minimum at their respective matching point, which lies at $(m-n).\varepsilon_F$.

4 - CONCLUSION -

We have derived a general iteration procedure to calculate m-particle n-hole level densities of any single particle Hamiltonian, including the Pauli principle. We have used this approach to derive analytical expressions for the semiclassical level densities up to 3-particles 3-holes of the isotropic Harmonic Oscillator, in the Thomas -Fermi approximation.

We learn that although the Pauli exclusion principle is more important at lower excitation energies and for higher particle-hole multiplicity, it does not change results very much on the logarithmic scale.

6.a)



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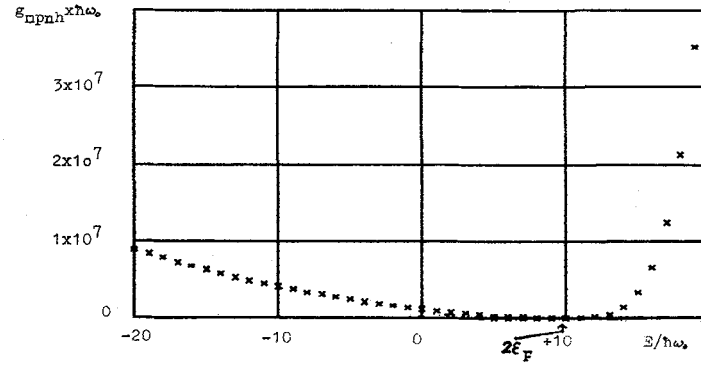

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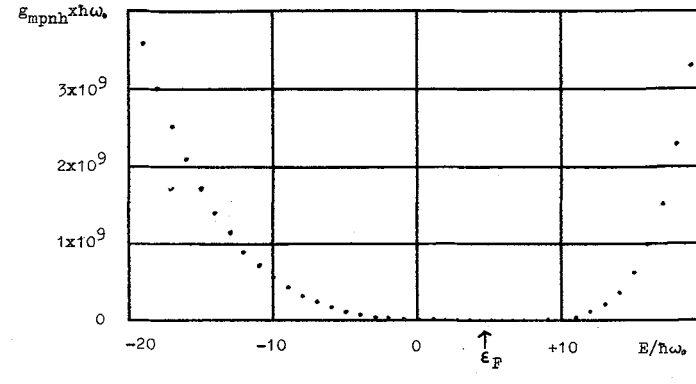

Fig.6 - Level density g_{mpnh} for $m \neq n$ and $m, n \neq o$.

a) $g_{2p1h}(E) + g_{1p2h}(-E)$ with minimum at $E = \varepsilon_F$

b) $g_{3p1h}(E) + g_{1p3h}(-E)$ with minimum at $E = 2\varepsilon_F$

c) $g_{3p2h}(E) + g_{2p3h}(-E)$ with minimum at $E = \varepsilon_F$

Note the different energy scales in each graph.

From the comparison of the n-particle n-hole density with a statistical level density formula we conclude, that one has to go beyond 3-particle 3-hole excitations also below an excitation energy of $4\hbar\omega_0$, in a semiclassical calculation.

Finally we have seen that the available phase space at the Fermi surface is depleted for particle-hole excitations with $m \neq n$ (except for the single particle).

We thank Mme C. Petit very much for typing the manuscript.

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